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Discrete element simulation and experimental study of powder spreading process in additive manufacturing

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ABSTRACT

Powders used in additive manufacturing (AM) are spread onto a compact layer of particles for sintering and this process is repeated layer by layer to form the final products. Spreading of rod-shaped particles in realistic AM settings is simulated using the discrete element method (DEM) to investigate the effects of particle shape and operating conditions on the bed quality, characterised by its surface roughness and solid volume fraction. It is discovered that larger particle aspect ratios, A_r, or higher spreader translational velocities result in a lower bed quality, i.e. a larger surface roughness and a smaller volume fraction. The surface roughness increases monotonically with A_r. However, the volume fraction exhibits a maximum at $A_r = 1.5$ for randomly packed powder beds that are formed by the roller type spreaders moving at low translational velocities. It is also found that a roller outperforms a blade spreader in terms of the quality of the prepared bed at the same operating conditions. The micro-structural analysis of the beds also shows particle alignment in response to the induced flow, which is qualitatively confirmed by a set of purposely-designed experiments. In addition, a shape segregation is documented for powders with mixed aspect ratios (A_r) such that particles with larger A_r tend to accumulate on the upper layers of the bed.

1. Introduction

Additive manufacturing has recently been exploited by various industries, such as automotive, aerospace and medical, as a novel production technology. Powder bed laser sintering (LS) or laser fusion is one of such promising AM techniques. It uses polymeric or metallic particles, heated to just below their melting temperature and spread on a fabrication piston to form a thin particle bed using a counter-rotating roller or a blade. A laser beam is then focused onto the bed and scans a raster pattern of a single layer of the final part. After sintering the fabrication piston lowers the part slightly and a new layer of powder is applied. The process is repeated until the product is successfully fabricated [1].

The technology offers substantial benefit for rapid production of prototypes and more recently for weight-sensitive/multi-functional final parts at small-volumes, with almost arbitrary complexity [2]. There is a growing demand for adoption of the technology. However, insufficient understanding of the multi-physics processes involved in the LS which comprise granular flow (spreading), heat transfer, phase change and surface phenomena, is hindering further development of the technology and introduction of new materials [3]. Such limitations result in expensive trial-and-error calibrations, uncertainty in the quality of final products and slow production rates due to interrupted builds.

The spreading process has a major impact on the characteristics and quality of the final product. The determining parameters are the solid volume fraction of the bed and smoothness of its surface since higher porosity or large roughness can lead to weaker bonding between layers and hence a poor mechanical performance. The importance of the layer smoothness and compactness has been demonstrated by Berretta et al. [4] using a new grade of Poly-Ether Ether Ketone (PEEK) in various spreading experiments. Ziegelmeier et al. [5] also reported strong connection between the powder volume fraction and the porosity of the sintered parts. They also demonstrated that the part's surface quality is highly dependant on the roughness of the powder bed.

The first analytical model, close to the LS method of operation, was developed by Johanson [6] to predict the behaviour of granular materials undergoing continuous shear between two rollers (see T-Dec et al. [7] for a review), and has been extended to compaction between a roller and a flat plate [8]. These models, however, treat

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powder beds as continuous media described by macroscopic conservation equations to calculate quantities such as stress distribution or bulk density within the bed. Therefore, the effects of particle shape and micro-structure on bed quality cannot be directly evaluated.

The development and performance of new material for the LS have also been the subject of a few experimental studies without linking to the spreading process itself. For instance, Wang et al. [9] studied the mechanical and thermal properties of graphite platelet reinforced PEEK (PEEK/GP). They showed that despite a higher porosity, the tensile strength of the composites is improved (maximum 36% improvement for 5 wt.% GP). Wang et al. [10] also studied the laser sintered glass bead filled Polyether ketone (GB/PEK) composites and showed up to 7% increase in hardness can be achieved without reducing its tensile strength.

Recently the DEM has been applied to the spreading problem to investigate the effects of particle level phenomena on the bed quality. Partelia and Pöschel [11] performed full device DEM simulations and found that the larger translational velocity of the roller and broader particle size distribution lead to larger surface roughness. Xiang et al. [12] simplified the process by considering an assembly of 4000 spherical particles undergoing three processes in their DEM simulations: random packing, layering and compression. Focusing on the effects of particle size distribution and considering mono-sized, bimodal and Gaussian distributions of spherical particles, they showed that the solid volume fraction increases with layer thickness regardless of the size distribution type.

In this paper, the spreading of *non-spherical* particles in AM is studied using DEM simulations. A commercial grade and two types of custom-milled PEK/PEEK powder particles are characterised experimentally. Based on these experiments rod-shaped particles are chosen for the simulations. The effects of spreading devices (roller or blade), their translational velocity and the bed thickness on the surface roughness and bed volume fraction are identified. It is found that a larger translational velocity generally reduces the bed quality and hence a lower value is suggested. This will however, adversely affect the production rate. In addition, it is found that the rollers produce powder beds with significantly better qualities and this is related to the contact dynamics between the spreader and the bed. The bed micro-structure in terms of particle orientation is analysed and an alignment phenomenon is observed and related to the bed response to the particle shape and the spreader velocity. Spreading experiments with rod particles are performed to qualitatively validate the particle alignment phenomenon. Finally, a mixture of rod-shaped particles with different aspect ratios is considered to study the shape segregation phenomenon. This analysis show that mixing particles with different shape/size distributions to control the bed quality may not be effective due to particle segregation in different layers of the bed.

It is also important to note that Parteli and Pöschel [11] earlier used similar DEM techniques to simulate the same process – admittedly with more realistic particle shapes. However, in this paper we have performed extensive parametric studies to characterise the process. Several adjustable parameters, available to device users, which are commonly used for tuning the process are considered and their effects on the bed quality are documented. In addition, we believe this is the first study that uses detailed micro-structural analysis to explain the complex dependence of bed quality on the aforementioned adjustable parameters and also on particle shape (at least for elongated particles).

2. Particle shape characterisation

PEK, PEEK and their composites have received significant attention in AM recently due to their good strength, stiffness, thermal, mechanical and chemical resistance [4,9,13-17]. This motivated us to characterise the shape of three different variations of these particles. This will also provide the basis for choosing the particle shapes in our numerical simulations. The commercial grade EOS HP3 PEK in addition to disk- and impact-milled 450G PEEK particles are considered. A cryogenic pulveriser (Powder King PKA-18) composed of a stationary and a rotating (at 30 Hz) disk with their gap set to 0.127 mm and its chamber cooled to −50 °C was used to disk-mill the grade 450G PEEK granules supplied by Victrex Plc. A 100 UPZII Universal Impact Mill (Hosokawa, Germany) operating at room temperature with a 2 mm sieve size and a blade rotation speed of 14,000 rpm was used for the impact milling.

The shape characterisation was performed in ImageJ software [18] analysing images obtained using a Scanning Electron Microscope (SEM) device (Hitachi S-3200N) under 20 kV acceleration voltage and with all samples coated with a 10 nm gold/palladium layer. Fig. 1 shows the results of this analysis. For the EOS HP3 PEK, both sphericity $\mathcal{S}$ and roundedness $\mathcal{R}$ are accumulated in the interval $[0.6, 0.8]$ showing properties of elongated particles with round edges. Aspect ratios are concentrated around $\mathrm{A}_r = 1.5$ with a notable tail extending to a $\mathrm{A}_r = 3.0$. Impact milled PEEK particles have the highest degree of sphericity $\mathcal{S} \approx 0.9$ and regularity with nearly 90% of particle having $\mathrm{A}_r \approx 2$. The disk-milled particles are quite irregular with the sphericity and roundedness spread between $0.2 < \mathcal{S} < 0.85$ and $0.15 < \mathcal{R} < 0.95$ respectively. However, accumulation on a diagonal line still characterises elongated particles and in fact the aspect ratio histogram shows a wide log-normal like distribution with mean value $\mathrm{A}_r \approx 2.5$ and a tail extending to $\mathrm{A}_r = 5$.

The results of these analyses show that elongated particles with a major axis and round edges are good approximations to the milled PEK/PEEK particles. Therefore, rod-shaped particle generated with a multi-sphere approach are chosen for the simulations (see Section 3.1).

3. Methodology

In this section the DEM technique is discussed first. Then the simulation and post-processing procedures are specified and their parameters are discussed in the relevant sections in detail. Nevertheless, a summary of important simulation/post-processing parameters is provided in Table 1 for reference.

3.1. Discrete element method

The Large-scale atomic/molecular massively parallel simulator (LAMMPS) code [19] is used for all the DEM simulations in this paper. Firstly, note that a distinction between a sphere and a particle is made since we will consider non-spherical particles created with a set of spheres. Therefore, a spherical/non-spherical particle is formed from one/or more spheres. A linear Hookean spring-dashpot contact force model is applied to each pair of spheres p and q whenever the two spheres overlap, i.e. when $\delta_{pq} = R_p + R_q - r_{pq} > 0$, where $r_{pq} = \| r_{pq,i} \| = \| r_{p,i} - r_{q,i} \|$[1], and $\| \bullet \|$ represents the Euclidean norm (magnitude) of any vector. In addition, R_k, $k \in \{p, q\}$, is the radius of the kth sphere and $r_{k,i}$ is the position vector of its centre of mass (CoM). The normal and tangential components of spring-dashpot force are given by

$$F^n_{pq,i} = \kappa_n \delta_{pq} n_{pq,i} - \gamma_n m^* v^n_{pq,i} \qquad (1)$$

$$F^t_{pq,i} = -\kappa_t u^t_{pq,i} - \gamma_t m^* v^t_{pq,i}, \qquad (2)$$

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[1] A tensor notation is adopted throughout this paper. For example $r_{p,i}$ with $i \in \{1, 2, 3\}$, is the position vector of sphere “p”.